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Is Multistep Necessary?

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In looking at simulations for the x-ray microscope the question "Is it necessary to use the multislice method to adequately model the transmission of x-rays through the target?" has been raised. Another question that has been raised is "Is it necessary to include diffraction effects in our simulations?" The purpose of this report is to lay these questions to rest.

The short answer to both of these questions is "No."

Multislice Method

The multislice method (also known as the beam propagation method (BPM))[1] is used to solve the paraxial wave equation. The paraxial wave equation is what the Helmholtz equation reduces to in the limit of small index of refraction deviations and small angular deviations. It lies in the middle ground between full wave simulation and ray tracing (a short wavelength limit). The BPM takes a region and cuts it into strips. The method then propagates a wavefront through the region one strip at a time. For each strip, the method first propagates the wavefront the width of the strip as if through free space (diffraction step), then the method applies a phase correction based on the index of refraction distribution in the strip (refraction step). In this way the method marches the wavefront through the region of interest.

Is it necessary to use the BPM to simulate x-ray microscopy of NIF targets? Or will ray tracing suffice? What role does diffraction play in the interaction between the x-ray beam and the object of interest?

Analytical Answer

An analytical answer to these questions is pointed to by the relation between computed tomography and diffraction tomography[2]. Given a region with resolvable features of size S, straight ray simulation for wavelength λ is appropriate for distances L such that

$$L << \frac{S^2}{2\lambda}$$

In our situation S is on the order of 1 micron, and λ is on the order of 2.5e-11 meters, so L must be much less than 2 cm. In the cases we're looking at, L is typically on the order of 3 mm, so we are at the upper edge of the reasonable range.

[1] M. D. Feit and J. A. Fleck, Jr., "Light propagation in graded-index optical fibers," Applied Optics, Vol. 17, No. 24, pp. 3990-3998, December 15, 1978.

[2] Greg Gbur and Emil Wolf, "Relation between computed tomography and diffraction tomography," J. Opt. Soc. Am. A, Vol. 18, No. 9, pp. 2132-2137, September 2001.

Simulation Testbed

Because 3 mm is less than 2 cm (but is it MUCH less?), we can be fairly certain that the BPM will not be necessary to simulate the x-ray microscopy process. To confirm this result we performed some simulations. We compared simulations based on straight ray propagation, BPM without diffraction, and full BPM propagation for the Ignition Double-Shell capsule NIF target. The target is shown in Figure 1. It should be noted that this simulation is of reduced dimension, so instead of a spherical capsule we have an infinite cylindrical capsule.

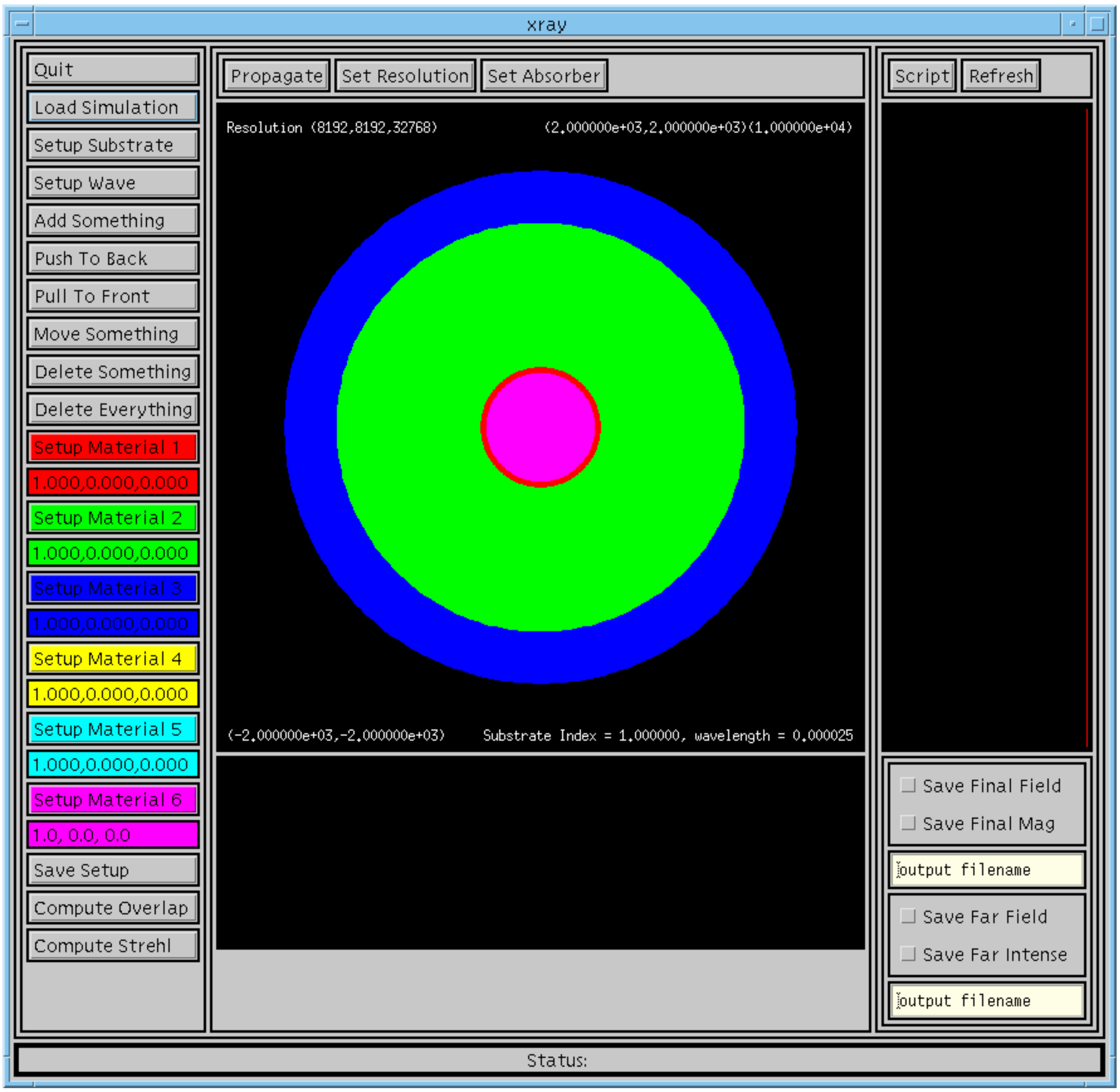

Figure 1. User interface to the straight_ray/BPM_no_diffraction/BPM code showing the IDS capsule NIF target prior to simulation.

In Figure 1 the pink region (of radius 0.337 mm) represents vacuum ($\delta = 0$, $\beta = 0$). The red region (of radius 0.372 mm) represents gold ($\delta = 3.55e{-6}$, $\beta = 1.64e{-7}$). The green region (of radius 1.275 mm) represents a carbon-hydrogen aerogel (δ and β effectively 0). The blue region (of radius 1.6 microns) represents a 0.997 Be +0.003 Cu alloy (δ = 3.83e-7, β = 9.921e-11). In all of the results that follow, we assume plane wave illumination with ~50 KeV x-rays and 150 mm propagation beyond the capsule.

Simulation Results

We simulated two capsule configurations in each of three ways (straight ray, BPM without diffraction, and full BPM). The two configurations were as follows: the capsule without defects, and the capsule with three 1 micron hemispheres of copper on the outer surface. The three hemispheres were centered on the back edge of the capsule (180 degrees), the top of the capsule (90 degrees), and in between (135 degrees).

Simulated x-rays from a plane wave source were propagated from one edge of the capsule to the other, then propagated through free space to a sensor 15 cm away. The result shown over the entire capsule is seen in Figure 2.

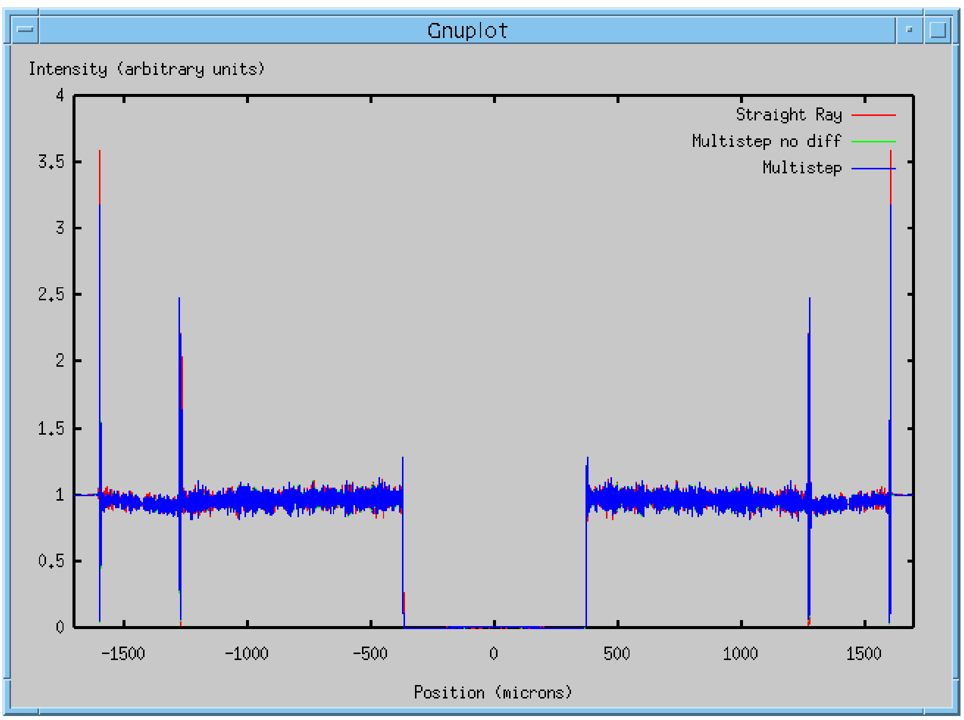

Figure 2. Results of the three propagation methods used on the smooth target. There is very little to distinguish the results of the three propagation methods.

Let us look more closely at some of the important regions in these results. First we will examine the transitions that do not involve the hemispherical bumps. The bottom of the capsule is shown in Figure 3, the aerogel/BeCu transition is shown in Figure 4, and the aerogel/Au transition is shown in Figure 5.

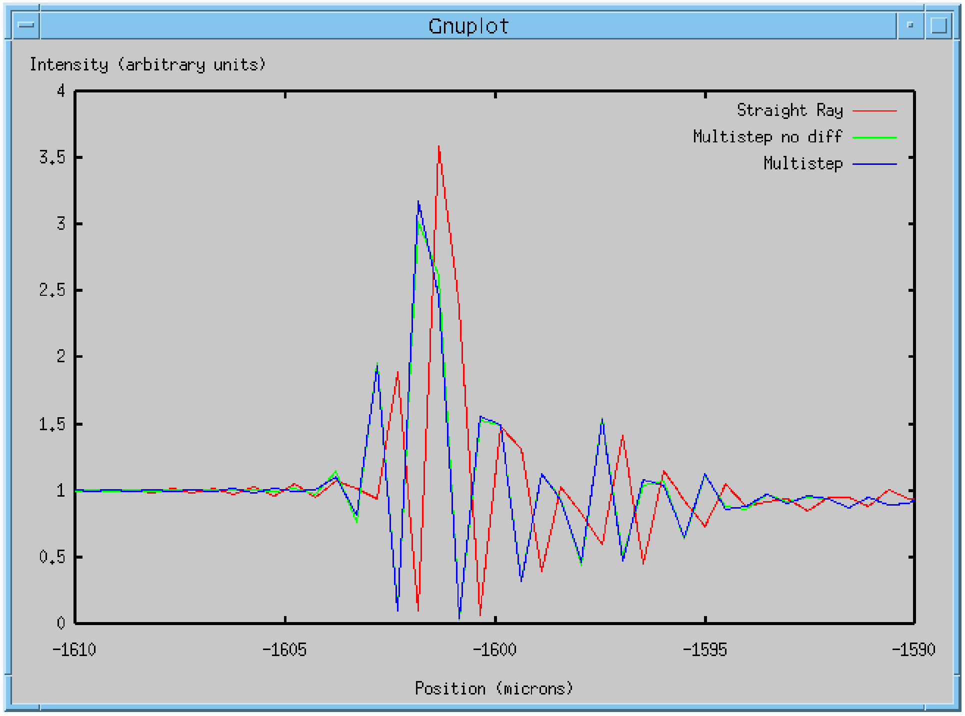

Figure 3. X-ray intensity distribution due to the bottom edge of the capsule. There is very little difference between the two BPM results, and a shift of about half a micron between the BPM results and the straight ray results.

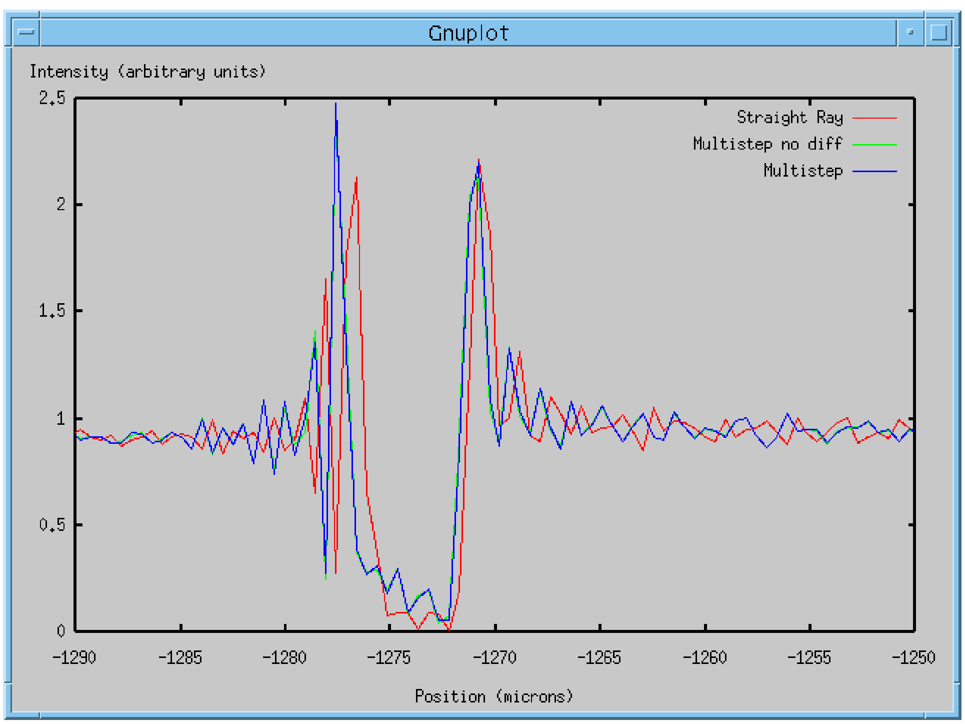

Figure 4. X-ray intensity distribution at the BeCu/aerogel interface. Once again the two BPM results lie atop one another and the straight ray results are shifted about half a micron.

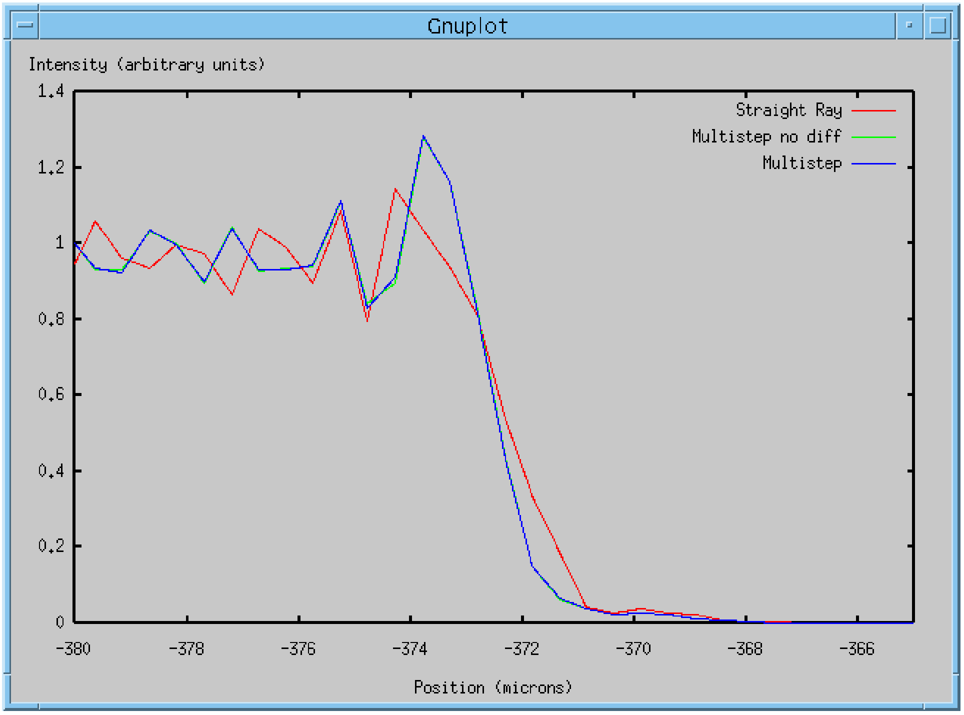

Figure 5. X-ray intensity distribution at the aerogel/Au interface. As in figures 3 and 4 the BPM methods lie atop one another.

Now we compare the regions with the bumps. Figure 6 shows the region around the bump at 180 degrees, figure 7 shows the region around the bump at 135 degrees, and figure 8 shows the region around the bump at 90 degrees.

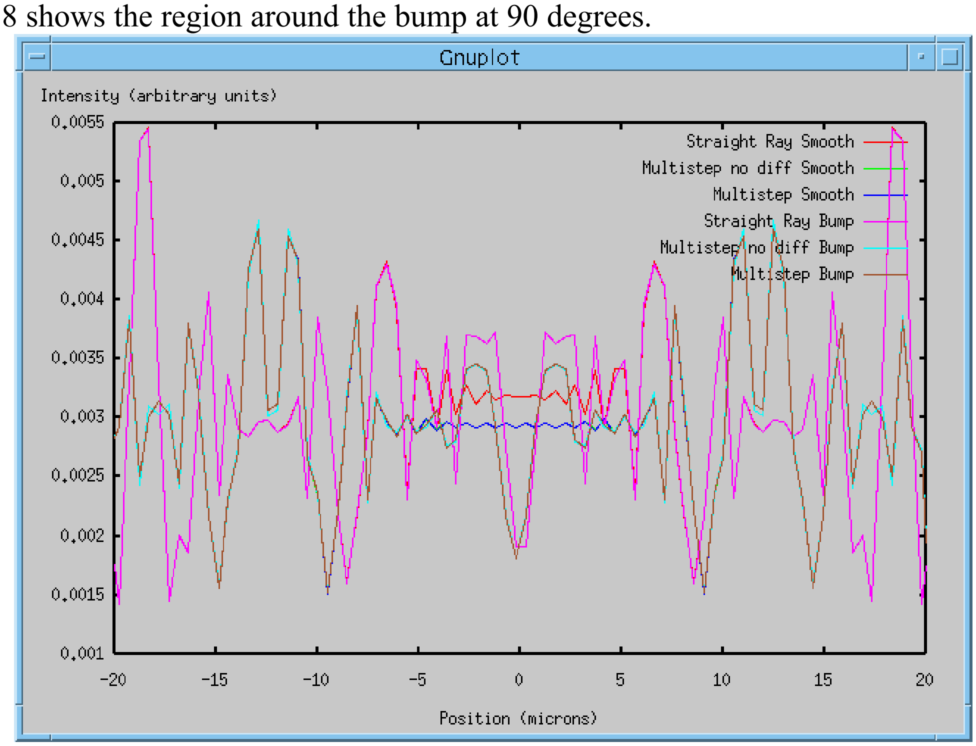

Figure 6. The region around 180 degrees. Away from the bump the straight ray projections lie atop one another. Away from the bump the BPM projections lie atop one another. The two methods generate different projections.

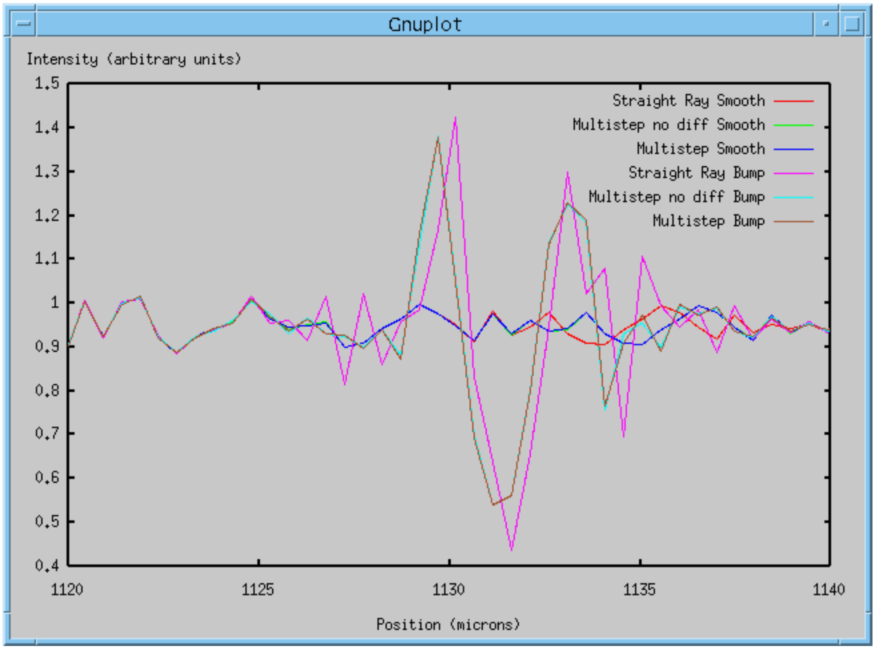

Figure 7. The region around the bump at 135 degrees. In this situation all of the simulations give similar results.

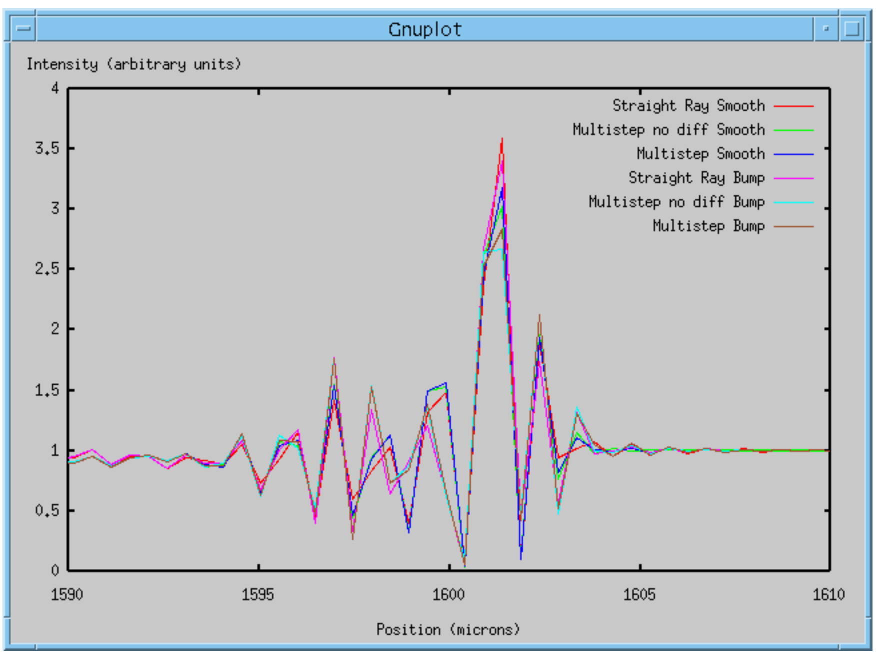

Figure 8. The region around the bump on the top of the capsule. It is difficult to see much difference between the corresponding smooth and bump results.

Confounding all of these results is the fact that in the actual x-ray microscope the x-ray source will not be coherent, so there will be a blur imposed on all of these results, washing out the fine details. There should be no distinction between the results of straight ray and multislice simulations under those conditions.